Recent Progress in Computational Methods Development for Pebble Bed Physics and System Modeling

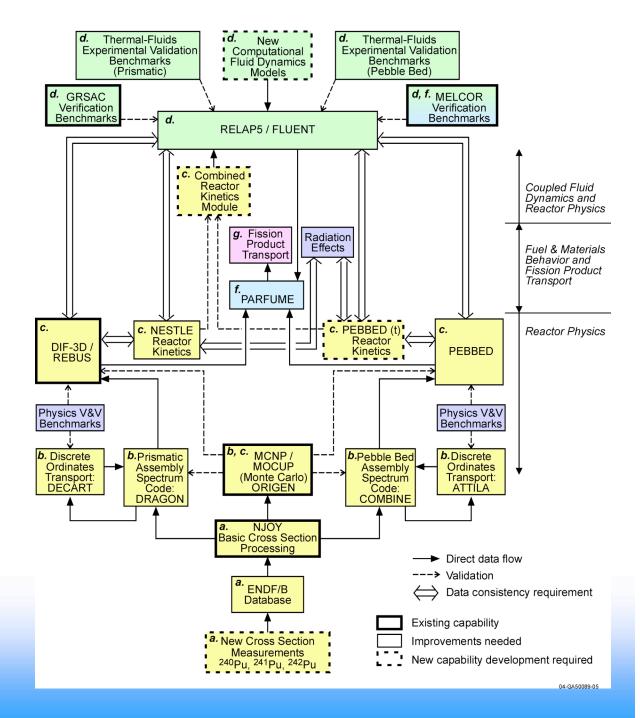
Abderrafi Ougouag, Hans Gougar, Joshua Cogliati, David Nigg, William Terry, Woo Yoon

> Ayman Hawari, NC State Kostadin Ivanov, Penn State Jan Kloosterman, TU Delft Farzad Rahnema, Ga Tech

> > December 8-9, 2005



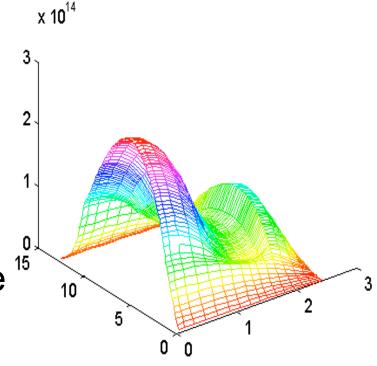
Proposed VHTR Code Suite





Pebble Bed Reactor Core Physics - Areas of Research and Development

- PEBBED pebble bed reactor fuel cycle analysis code
- Coupled-Code Development and Crosssection Generation
- Material-Neutronics Interface



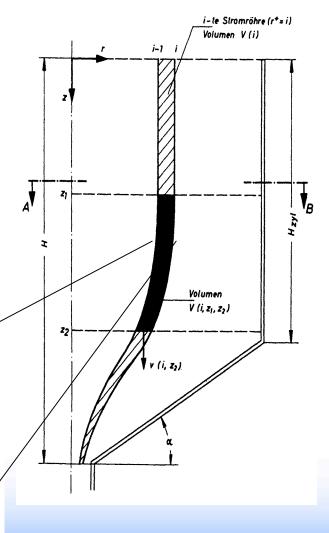


The PBR Fuel Management Problem

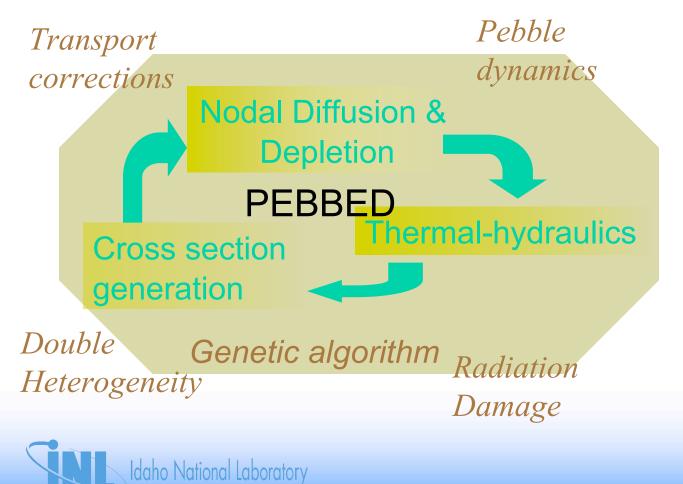
- Fuel flows along streamlines (deterministic component)
- Stochastic component leads to uncertainty
- Partially burned pebbles are recirculated until spent
- Long mean free path, high burnup, harder spectrum

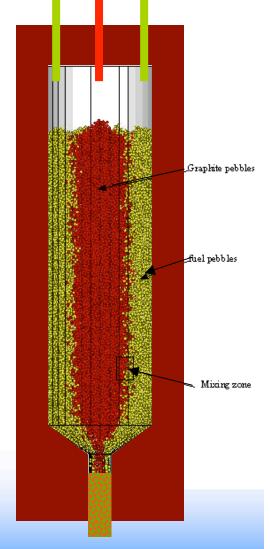
LWR methods & codes cannot easily be applied

Idaho National Laboratory



Pebble Bed Reactor Core Physics - Areas of Research and Development

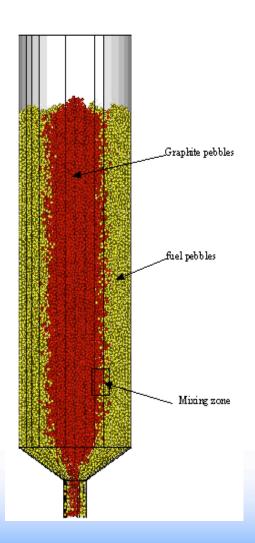




PEBBED

- Equilibrium Fuel Cycle Analysis of Pebble Bed Reactors
- Finite Difference or Nodal Diffusion
- Low-order thermal-hydraulic modules for normal and accident temperature estimation or THERMIX for accuracy
- Thermal cross section feedback via table lookup or direct calls to a spectrum module
- Arbitrary pebble recirculation schemes can be modeled
- Genetic Algorithm for core geometry and fuel loading optimization



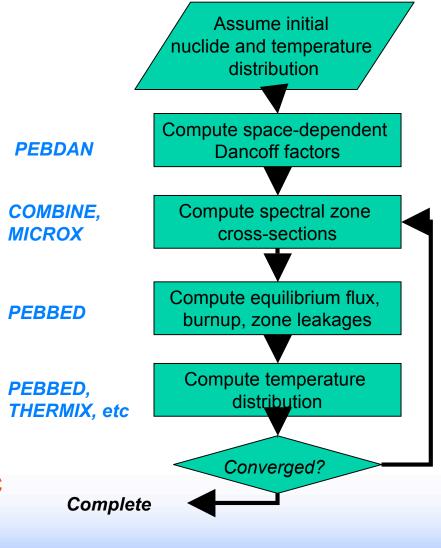


Cross sections for TRISO-based Fuel

• 2 or 3 levels of heterogeneity Pebble Bed Core Randomness in fuel lattice Low-energy resonances in minor Pebble actinides Uncertainty in burnup history Long mean free path **FUEL PARTICLES** particle Compact Idaho National Laboratory **Block** Prismatic Core

Current Efforts

- Development of Analytical Nodal Diffusion Solver
- Transport Corrections for non-diffusive regions
- Improved Cross-section generation with COMBINE
- Transient Analysis with NEM-THERMIX
- Computational Pebble Flow Dynamics
- Calculation of Displacement Threshold Energy/Neutronic Effects of Radiation
 - Damage and Annealing



Integrated PBR Fuel Cycle Analysis

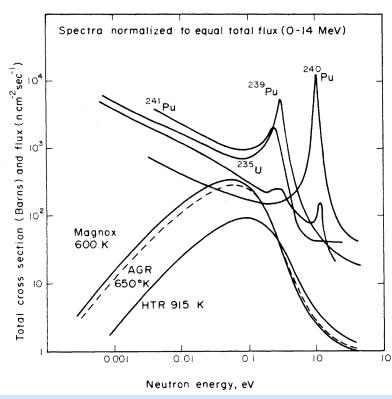
COMBINE (ENDF/B v6) Developments

- Proper treatment of low energy resonances, energy dependent bucklings, quantum levels in resolved resonances, lumped fission parameters)
- Double-heterogeneity with a new method for computation of spatially-dependent Dancoff factors
- Efficient (on-line) coupling to PEBBED

Outstanding Issues

- Leakage effect between nodes
- Proper generation of cross
 sections in non-multiplying media (reflectors, voids)

Integrated Cross-section Generation

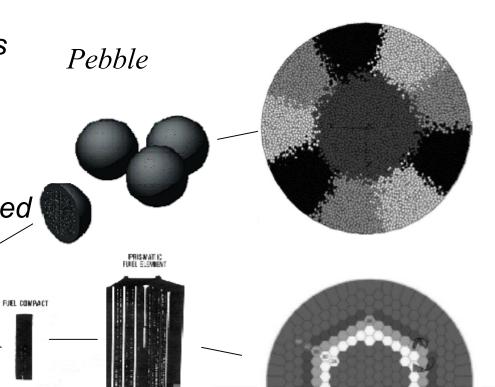


Dancoff Factors for VHTR Fuel

Builds on previous work by Bende & Kloosterman but with a rigorous treatment of randomness and spatial effects (with cooperation of Prof. Kloosterman of TU Delft)
Particle (intra-pebble) and

 Particle (intra-pebble) and geometry-dependent interpebble Dancoff factors computed

particle





Block

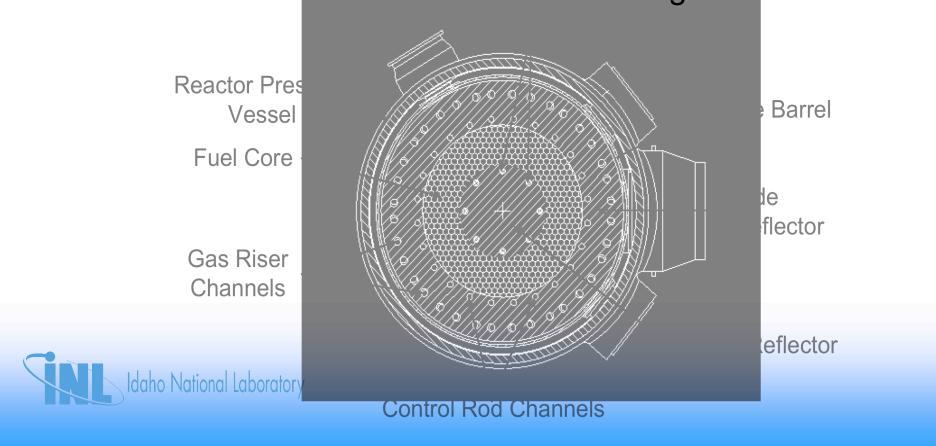
Compact

Prismatic Core

Pebble Bed Core

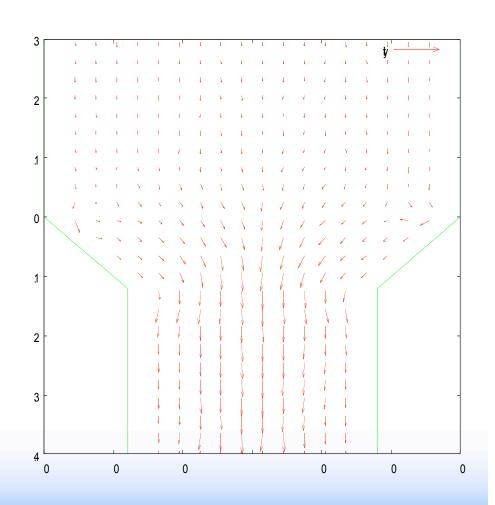
Integrated transport treatment for nondiffusive nodes

- Response Matrix (transport) approach under investigation (Georgia Institute of Technology)
- Preliminary results look promising an RZ transient diffusion solver with embedded RM is being tested



Pebble Flow Simulation

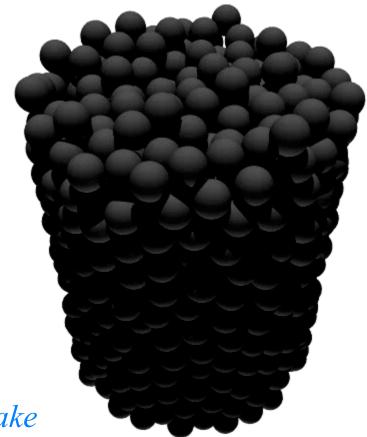
- Hard particle dynamics simulation of core loading and settling
- Variable packing fraction and pebble flow simulated but not validated for graphite
- Dynamics of pebble flow to drive time-dependent fuel loading analysis capability (Approach to Asymptotic)
- Experimental validation and determination of parameters are needed





Pebble Settling during a Seismic

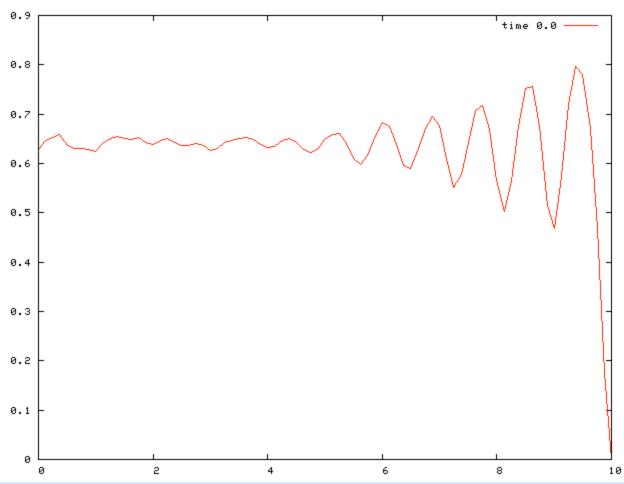
Event



1000 pebbles in vat Mercalli X horizontal quake

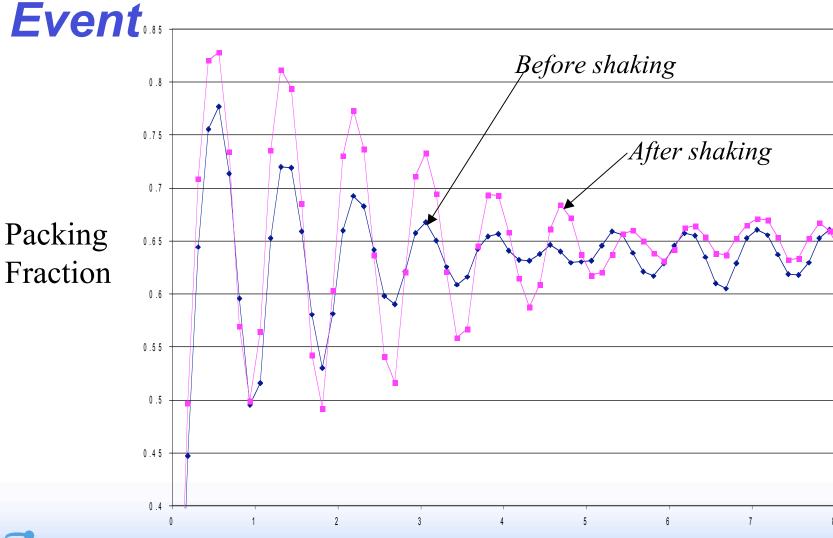


Pebble Settling during a Seismic Event





Pebble Settling during a Seismic





Distance (in pebble diameters)

Material-Neutronics Interface – modeling radiation damage and its effects on core dynamics

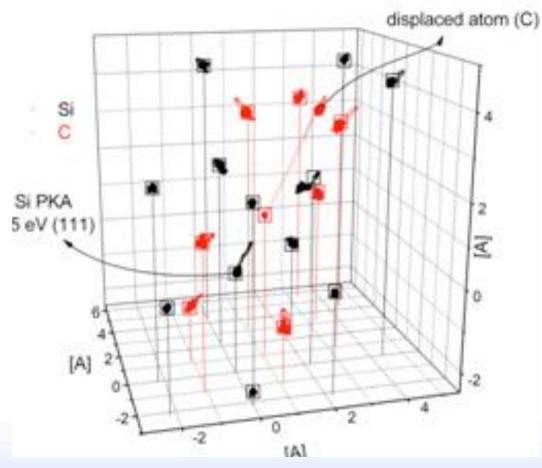
- Molecular dynamic simulation of radiation damage in graphite and SiC
- Calculation of scattering cross sections in damaged crystals
- Calculation of threshold energy and displacement kerma cross sections at prototypical temperatures
- Modeling of damage to assess effects of annealing on transient behavior (thermal conductivity recovery – thermal scattering law changes)

$$E = \frac{1}{2} \sum_{i \neq j} \left\{ f_c(r_{ij}) \left[f_R(r_{ij}) + b_{ij} f_A(r_{ij}) \right] \right\}$$

$$f_c(r_{ij}) = \begin{cases} 1 & , r_{ij} < R_{ij} \\ \frac{1}{2} \left\{ 1 + \cos \left[\pi \frac{\left(r_{ij} - R_{ij} \right)}{\left(S_{ij} - R_{ij} \right)} \right] \right\} & , R_{ij} < r_{ij} < S_{ij} \\ 0 & , S_{ij} < r_{ij} \end{cases}$$

$$|C_{ij}| = \begin{cases} 1 & , r_{ij} < R_{ij} \\ \frac{1}{2} \left\{ 1 + \cos \left[\pi \frac{\left(r_{ij} - R_{ij} \right)}{\left(S_{ij} - R_{ij} \right)} \right] \right\} & , R_{ij} < r_{ij} < S_{ij} \end{cases}$$

Dynamic modeling of radiation damage

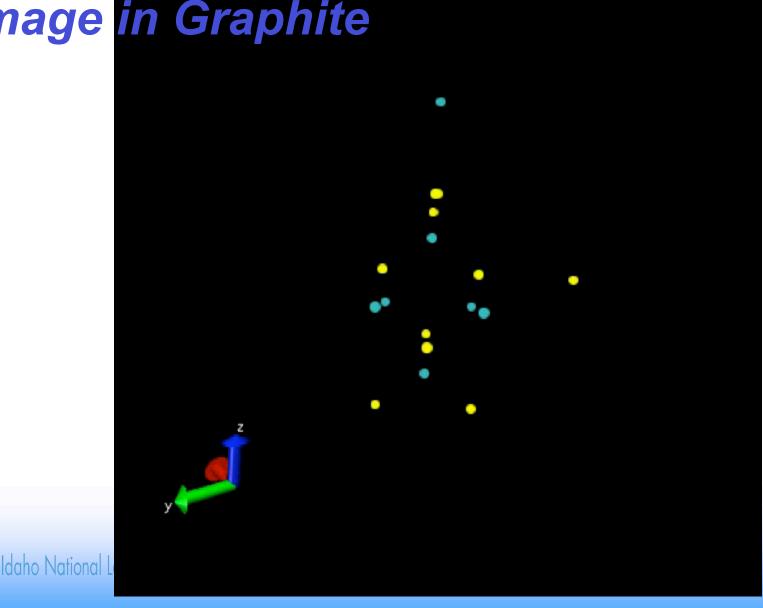


MDCASK model of atomic movement in SiC



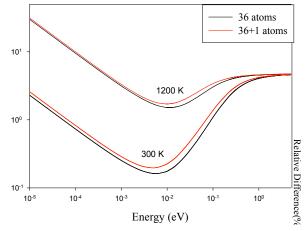
Kinetic Modeling of Irradiation

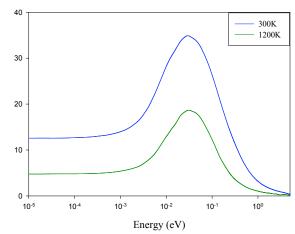
Damage in Graphite



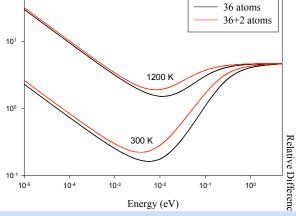
Effect of radiation damage on scattering cross section

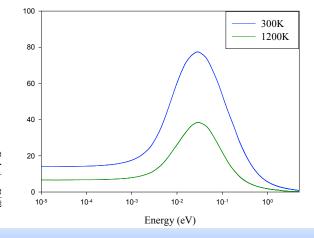
1 interstitial atom





2 interstitial atoms



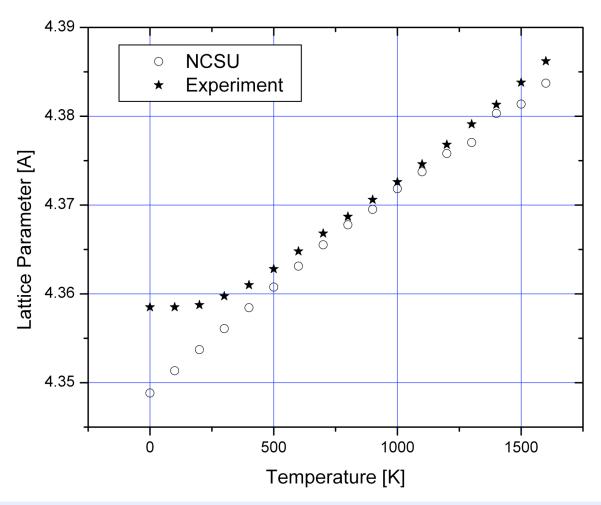




Thermal inelastic scattering cross section (b)

Relative Difference (%)

Prediction of lattice parameters





Summary

- PEBBED for state-of-the-art PBR analysis and design
 - Advanced optimization
 - Nodal Diffusion
- Coupled-Code Development and Implementation
 - NEM-THERMIX (thermal)
 - COMBINE (cross sections)
- Radiation effects on Core Dynamics
- 2006 Validation and benchmarking of results

